

Sulfur-functionalized Mesoporous Carbons as Sulfur Hosts in Li–S Batteries: Increasing the Affinity of Polysulfide Intermediates to Enhance Performance

Kimberly A. See,^{†,‡,¶} Young-Si Jun,^{†,‡} Jeffrey A. Gerbec,^{†,§} Johannes K. Sprafke,[†]
Fred Wudl,^{†,||} Galen D. Stucky,^{†,‡,||,¶} and Ram Seshadri^{*,†,‡,||,¶}

Mitsubishi Chemical – Center for Advanced Materials, University of California, Santa Barbara, CA 93106, USA., Department of Chemistry and Biochemistry, University of California, Santa Barbara, CA 93106, USA., Materials Research Laboratory, University of California, Santa Barbara, CA 93106, USA., Mitsubishi Chemical USA, Inc., Chesapeake, VA 23320, USA., and Materials Department, University of California, Santa Barbara, CA 93106, USA.

E-mail: seshadri@mrl.ucsb.edu

^{*}To whom correspondence should be addressed

[†]Mitsubishi Chemical – Center for Advanced Materials, University of California, Santa Barbara, CA 93106, USA.

[‡]Department of Chemistry and Biochemistry, University of California, Santa Barbara, CA 93106, USA.

[¶]Materials Research Laboratory, University of California, Santa Barbara, CA 93106, USA.

[§]Mitsubishi Chemical USA, Inc., Chesapeake, VA 23320, USA.

^{||}Materials Department, University of California, Santa Barbara, CA 93106, USA.

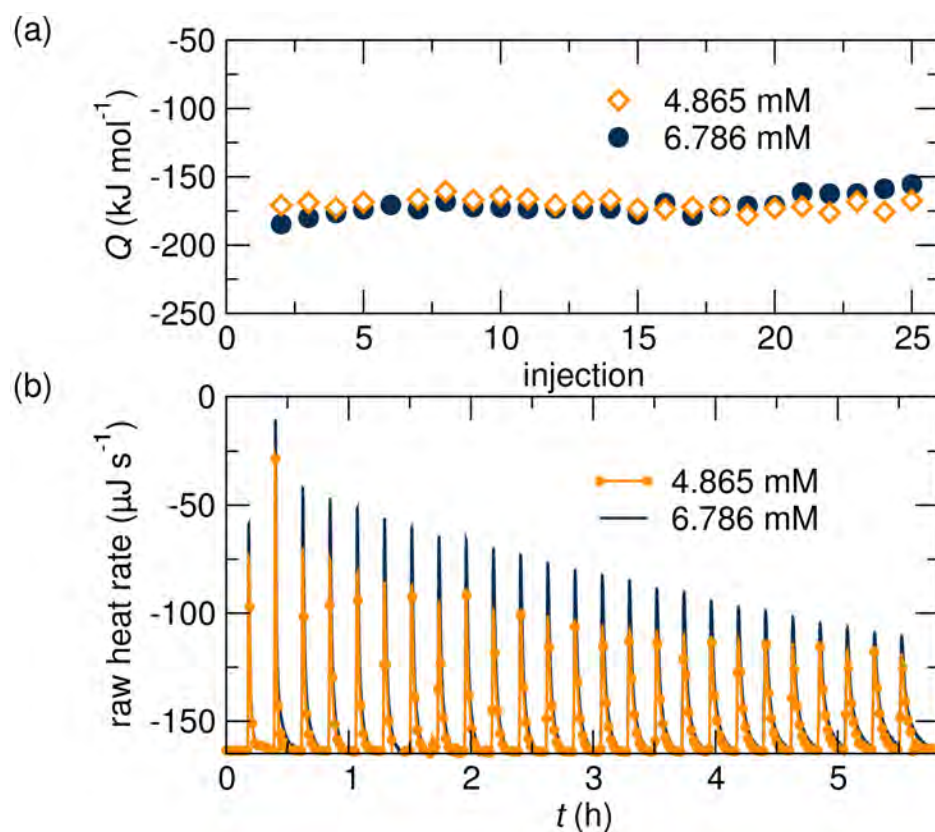


Figure S 1: The heat of dilution of “ Li_2S_6 ” into 1,3-dioxolane (DOL) as determined by isothermal titration calorimetry. 4.865 mM and 6.786 mM solutions of “ Li_2S_6 ” in DOL were titrated into DOL in order to determine the background heat of dilution. These background heats were then subtracted injection by injection from subsequent ITC experiments in order to deconvolute the heat due to dilution and that due to the interaction of “ Li_2S_6 ” with the carbons.

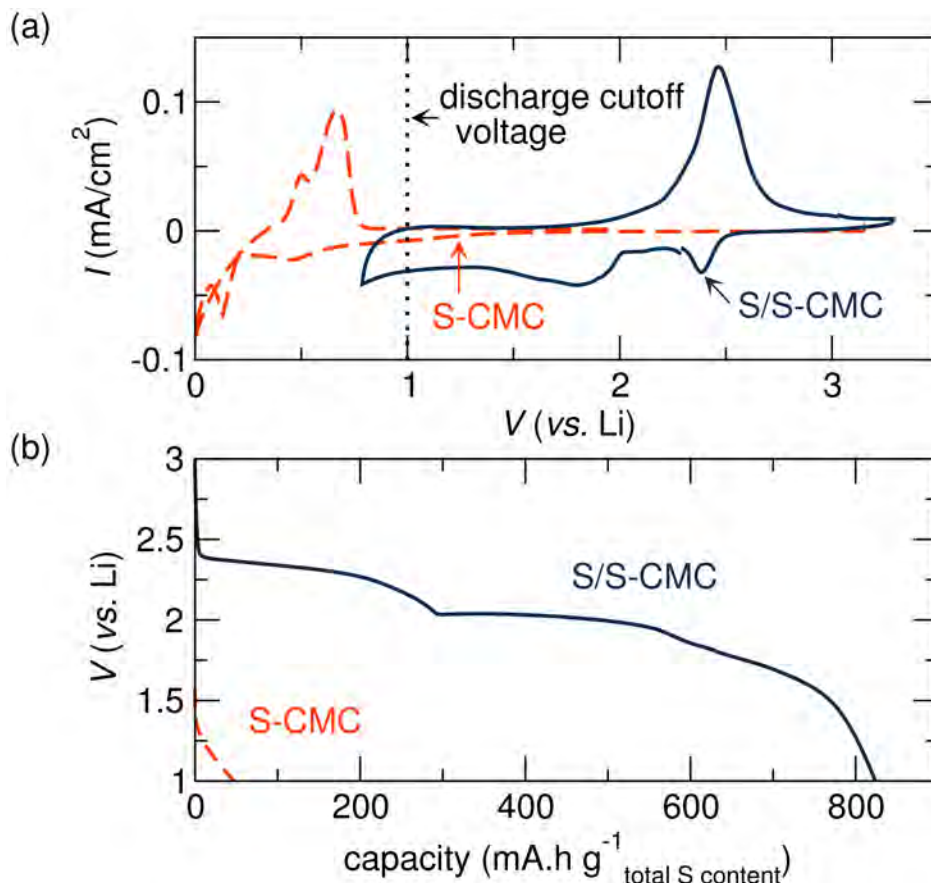


Figure S 2: (a) Cyclic voltammetry of sulfur-functionalized cubic mesoporous carbon (S-CMC) and sulfur infiltrated sulfur-functionalized cubic mesoporous carbon (S/S-CMC) vs. a Li anode in 1 M LiTFSI in ethyl methyl sulfone electrolyte at 0.05 mV/s shows negligible current due to the sulfur functionality above 1 V indicating that the sulfur moieties present in the carbon are not participating in the charge storage above 1 V. The reduction events below 1 V are due to carbon and Li deposition at low potentials. (b) The galvanostatic discharge profile of S-CMC compared with S/S-CMC. Without sulfur infiltration, the S-CMC shows negligible capacity between the voltage ranges probed while cycling the Li-S cell (1.0 V – 2.6 V).